

Glycine, 2-cyclohexyl-N-isobutoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C29H55NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-33-28(31)27(26-21-12)
InchiKey: OZSTZPBIPQZJS-UHFFFAOYSA-N
Formula: C29H55NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)OCC(C)C)C1CCCCC1
Mol. weight [g/mol]: 481.75

Physical Properties

Property code	Value	Unit	Source
gf	-165.58	kJ/mol	Joback Method
hf	-1034.26	kJ/mol	Joback Method
hfus	66.33	kJ/mol	Joback Method
hvap	104.55	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.342		Crippen Method
mcvol	433.470	ml/mol	McGowan Method
pc	740.03	kPa	Joback Method
rinpol	3154.00		NIST Webbook
rinpol	3154.00		NIST Webbook
tb	1084.34	K	Joback Method
tc	1342.78	K	Joback Method
tf	590.95	K	Joback Method
vc	1.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1599.06	J/mol×K	1084.34	Joback Method
cpg	1618.43	J/mol×K	1127.41	Joback Method
cpg	1635.32	J/mol×K	1170.49	Joback Method
cpg	1649.84	J/mol×K	1213.56	Joback Method
cpg	1662.09	J/mol×K	1256.63	Joback Method
cpg	1672.18	J/mol×K	1299.71	Joback Method
cpg	1680.23	J/mol×K	1342.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383106&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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